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Superscripts

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Solubility and Diffusivity of Acid Gases (CO₂, N₂O) in Aqueous Alkanolamine Solutions

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Solubility and diffusivity of N₂O and CO₂ in water were determined as a function of temperature from the results published in the open literature, and new data were measured in the present work. The solubility of N₂O in several aqueous alkanolamine (DEA, DIPA, DMMEA, and DIPA) solutions at various temperatures was measured and correlated over a wide range of conditions. For both the diffusivity of N₂O and the alkanolamine in aqueous alkanolamine solutions a modified Stokes-Einstein relation was derived. With the aid also of the "N₂O analogy" the diffusivity of CO₂ in these solutions can be estimated.

1. Introduction

Alkanolamines have become one of the most important classes of chemicals for the removal of the acid gas components H₂S and CO₂ from several types of gases. Frequently, aqueous solutions are applied; however, mixtures of water and a nonaqueous solvent are also used (e.g., Shell-Sulfinol process (1)). Diisopropanolamine (DIPA), methyldiethanolamine (MDEA), monoethanolamine (MEA), and diethanolamine (DEA) are examples of well-known and industrially important amines (Kohl and Riesenfeld (1)).

For the design of suitable gas-liquid contactors for the above-mentioned gas-treating processes it is necessary that the mass-transfer rates can be calculated accurately. Besides needed information on the mass-transfer coefficients, gas-liquid contact area, and reaction kinetics, data are also needed on the fundamental physicochemical properties like the solubility and the diffusivity of the acid gas components in the various solutions. However, due to the chemical reaction that occurs in the solution, it is not possible to obtain information directly on these properties and therefore they must be estimated from corresponding data of more or less similar nonreacting gases.

In view of the similarities with regard to configuration, molecular volume, and electronic structure, N₂O is often used as nonreacting gas to estimate the properties of CO₂. Laddha et al. (2) investigated the solubility of N₂O and CO₂ in aqueous solutions of organic compounds that are nonreacting with respect to both solutes and organic alcohols that have a somewhat similar structure to MEA and DEA. From this work it was concluded that the ratio of the solubilities remained constant for the various solutions and that the "N₂O analogy" may be applied to estimate the solubility of CO₂ in aqueous alkanolamine solutions according to the equation

$$(\text{solubility of CO}_2) = C_1(\text{solubility of N}_2\text{O}) \quad (1)$$

with

$$C_1 = (\text{solubility of CO}_2 \text{ in water})/(\text{solubility of N}_2\text{O in water}) \quad (2)$$

Sada et al. (3, 4) mentioned earlier that the N₂O analogy could be used to obtain information on the solubility of CO₂ and also considered that a relation similar to eq 1 could be applied to estimate the diffusivity of CO₂. From Sada et al.'s (3, 4) results, however, it was not possible to derive a general correlation to calculate the diffusivity of N₂O (or CO₂) in aqueous alkanolamine solutions. Versteeg (5) recently published additional data on the diffusivity of N₂O in aqueous alkanolamine solutions, and these data showed a good agreement with the results of Sada et al. (4) although for DEA a substantial deviation occurred. Nevertheless, it may be possible to obtain a general (e.g., a modified Stokes-Einstein relation) relation that is able to calculate the diffusivity.

Halmour and Sandall (6) studied the absorption of CO₂ and N₂O in aqueous MDEA solutions at various temperatures in a laminar liquid jet. At very short contact times the absorption of CO₂ can be considered as physical absorption without any enhancement due to the chemical reaction and therefore it was possible to verify for this particular solution the N₂O analogy for both solubility and diffusivity combined in the physicochemical parameter $mD^{1/2}$. From their results it could be concluded that for aqueous MDEA solutions the "analogy" holds.

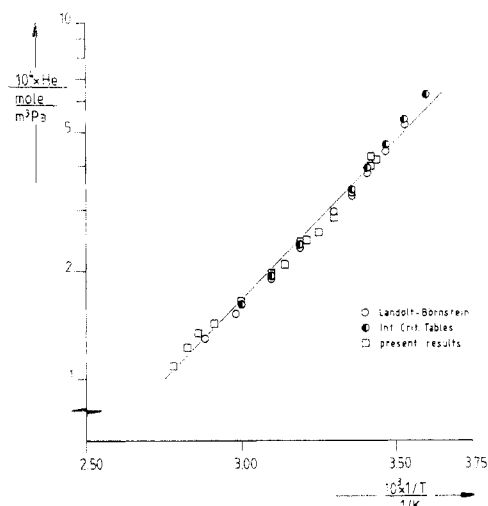
In the present work new data on both solubility and diffusivity of N₂O in aqueous alkanolamine solutions at various temperatures will be presented and for CO₂, using the N₂O analogy, both properties can be estimated. The available data of the solubility and diffusivity of CO₂ and N₂O in water published in the open literature are summarized in combination with these new data.

2. Solubility

2.1. Experimental Procedure. The solubility was measured in a glass vessel with a volume of $1.05 \times 10^{-3} \text{ m}^3$ which was filled with a calibrated volume ($4.02 \times 10^{-4} \text{ m}^3$) of solution. In each experiment the solution was degassed by means of evacuation of the equilibrium vessel and the contents were held under vacuum until bubbles of air ceased to be evolved by the liquid and then the vapor-liquid equilibrium was established. Equilibrium pressure was recorded by a pressure transducer. The appropriate gas was then fed to the vessel until a arbitrary

Table I. Solubility of CO₂ in Water at Various Temperatures (Present Study)

temp, K	solubility, mol·mol ⁻¹	10 ⁴ HE, mol·m ⁻³ ·Pa ⁻¹
291	0.980	4.05
292	1.006	4.15
292	0.943	3.89
293	0.925	3.80
298	0.833	3.37
298	0.815	3.29
303	0.706	2.80
308	0.648	2.54
311.4	0.631	2.44
313	0.617	2.37
313.4	0.619	2.38
318	0.544	2.06
323	0.520	1.94
333	0.451	1.63
343.5	0.401	1.40
350.2	0.385	1.32
355.2	0.357	1.20
360.1	0.322	1.08

**Figure 1.** Solubility of CO₂ in water as a function of temperature.

pressure was reached ($P \leq 10^5$ Pa), which was also recorded. Then the vessel was closed and the magnetic stirrer was started to agitate the liquid and after the equilibrium pressure was reached the solubility could be calculated, based on Henry's law according to

$$m = \frac{HE}{RT} = \frac{(P^{\text{int}} - P^{\text{eq}}) V_{\text{gas}}}{P^{\text{eq}} V_{\text{liq}}} \quad (3)$$

where m is a kind of dimensionless solubility defined as the ratio of the liquid-phase concentration to the gas-phase concentration of the solute at equilibrium conditions. The reproducibility between the various experiments was always within 3%.

The solutions were prepared from commercial grade amines, purity $\geq 98\%$, and distilled water. The composition of the aqueous solution was determined by volumetric titration as described by Blauwhoff et al. (7).

2.2. Solubility of CO₂ and N₂O in Water. The solubility data for CO₂ from the present work are presented in Table I. These results are compared in Figure 1 with the data published in the open literature (8, 9). The effect of the reaction between CO₂ and H₂O on the solubility is very small and can therefore be neglected (10). From Figure 1 it can be seen that the solubility of CO₂ in water can be calculated as a function of temperature according to

$$HE_{\text{CO}_2} = 3.54 \times 10^{-7} \exp(2044/T) \text{ mol} \cdot \text{m}^{-3} \cdot \text{Pa}^{-1} \quad (4)$$

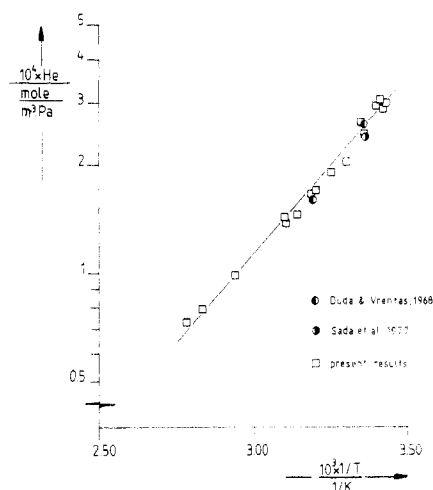
where HE is the Henry's law coefficient.

Table II. Solubility of N₂O in Water at Various Temperatures

temp, K	solubility, mol·mol ⁻¹	10 ⁴ HE, mol·m ⁻³ ·Pa ⁻¹	ref
291.2	0.725	2.99	present study
292	0.698	2.87	present study
292.9	0.731	3.00	present study
293	0.711	2.92	present study
298	0.599	2.42	present study
298	0.602	2.43	Sada et al. (4)
298	0.634	2.56	Duda and Vrentas (16)
298	0.597	2.41	Joosten and Danckwerts (17)
298.6	0.656	2.65	present study
302.9	0.509	2.02	present study
308	0.484	1.90	present study
312.9	0.439	1.69	present study
313	0.429	1.65	present study
313	0.419	1.61	Duda and Vrentas (16)
318	0.377	1.43	present study
322.6	0.375	1.40	present study
322.9	0.362	1.35	present study
340	0.273	0.97	present study
353	0.228	0.78	present study
359.4	0.212	0.71	present study

Table III. Solubility of N₂O in Aqueous DMMEA Solutions at 293 K

[DMMEA], mol·m ⁻³	solubility, mol·mol ⁻¹	[DMMEA], mol·m ⁻³	solubility, mol·mol ⁻¹
324	0.677	1591	0.630
611	0.680	1968	0.604
830	0.667	2049	0.586
1218	0.651	2388	0.585

**Figure 2.** Solubility of N₂O in water as a function of temperature.

In Table II the data of the solubility of N₂O from the present work in combination with literature results are presented, and from Figure 2 the solubility of N₂O can be calculated with

$$HE_{\text{N}_2\text{O}} = 1.17 \times 10^{-7} \exp(2284/T) \text{ mol} \cdot \text{m}^{-3} \cdot \text{Pa}^{-1} \quad (5)$$

From eq 3 and 4 the constant C_1 in eq 1 can be obtained as a function of the temperature:

$$C_1 = 3.04 \exp(-240/T) \quad (6)$$

For 298 K, $C_1 = 1.36$ which is in excellent agreement with the value 1.37 reported by Laddha et al. (2).

2.3. Solubility of N₂O and CO₂ in Aqueous Alkanolamine Solutions. The solubility of N₂O was measured for aqueous solutions of dimethylmonoethanolamine (DMMEA) at 293 K, DEA at 298 K, and for both DIPA and MDEA at various temperatures. The results are presented in Table III (DMMEA), Table IV (DEA), Table V (DIPA), and Table VI (MDEA). For DEA and

Table IV. Solubility of N₂O in Aqueous DEA Solutions at 298 K

[DEA], mol·m ⁻³	solubility, mol·mol ⁻¹	[DEA], mol·m ⁻³	solubility, mol·mol ⁻¹
449	0.595	2290	0.542
1397	0.564	2313	0.556
1418	0.559	2360	0.531
1556	0.573	2389	0.553
2026	0.565	3081	0.535

Table V. Solubility of N₂O in Aqueous DIPA Solutions at Various Temperatures

[DIPA], mol·m ⁻³	temp, K	solubility, mol·mol ⁻¹	[DIPA], mol·m ⁻³	temp, K	solubility, mol·mol ⁻¹
330	293	0.661	1978	298	0.505
346	293	0.684	2070	298	0.487
505	293	0.668	2091	298	0.501
751	293	0.641	2105	298	0.468
1025	293	0.669	2145	298	0.509
1170	293	0.613	2390	298	0.485
1218	293	0.614	2393	298	0.470
1436	293	0.624	2508	298	0.464
1466	293	0.590	2733	298	0.461
1545	293	0.561	2781	298	0.442
1725	293	0.575	2826	298	0.435
1978	293	0.567	4056	298	0.414
2222	293	0.522			
2390	293	0.539	346	308	0.452
2890	293	0.530	1025	308	0.454
3310	293	0.508	1545	308	0.432
3360	293	0.471	1978	308	0.421
3450	293	0.497	2390	308	0.411
286	298	0.607	346	318	0.383
292	298	0.597	1025	318	0.354
346	298	0.571	1545	318	0.437
696	298	0.565	1978	318	0.367
724	298	0.569	2390	318	0.366
952	298	0.556	346	333	0.319
1025	298	0.570	1025	333	0.313
1545	298	0.544	1545	333	0.313
1758	298	0.510	1978	333	0.322
1901	298	0.497	2390	333	0.314

DIPA at 298 K a good agreement exists with the data published by Sada et al. (3, 4).

The solubility of CO₂ can be estimated by using eq 1 and 5 and the solubility of N₂O. The experimental solubilities of N₂O were fitted to a polynomial function according to

$$m = a_0 + a_1[\text{amine}] + a_2[\text{amine}]^2 + \dots + a_n[\text{amine}]^n \quad (7)$$

and in Table VII the polynomial coefficients are presented. Therefore the solubility of CO₂ can be estimated from eq 1, 5, and 6 over a wide range of conditions.

3. Diffusivity

3.1. Experimental Method. The diffusivity was determined from physical absorption experiments in a stirred vessel operated with a horizontal gas-liquid interface, which appeared visually to be completely smooth. The experimental method applied was identical with that developed recently by Versteeg et al. (5).

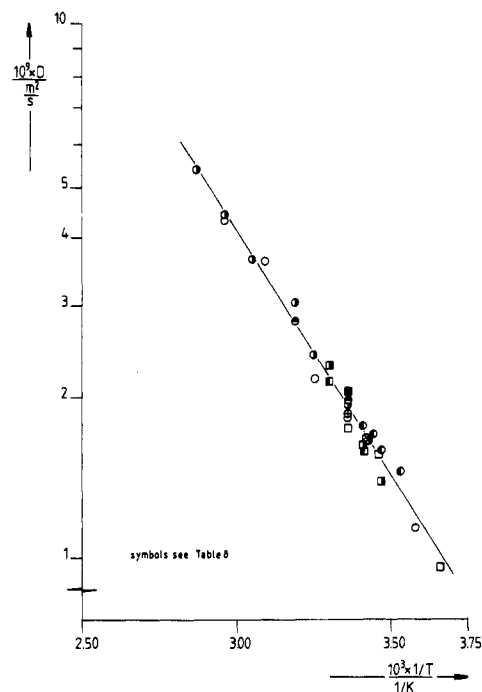
3.2. Diffusivity of CO₂ and N₂O in Water. In Table VIII the data published in the open literature on the diffusivity of CO₂ in water are summarized and presented graphically as a function of temperature in Figure 3. The diffusivity of CO₂ in water can be calculated with

$$D_{\text{CO}_2} = 2.35 \times 10^{-6} \exp(-2119/T) \text{ m}^2\cdot\text{s}^{-1} \quad (8)$$

In Table IX the data published in the open literature on the diffusivity of N₂O in water are summarized together with the

Table VI. Solubility of N₂O in Aqueous MDEA Solutions at Various Temperatures

[MDEA], mol·m ⁻³	temp, K	solubility, mol·mol ⁻¹	[MDEA], mol·m ⁻³	temp, K	solubility, mol·mol ⁻¹
348	393	0.683	1251	308	0.467
415	293	0.679	1320	308	0.465
716	293	0.665	1457	308	0.462
793	293	0.661	1509	308	0.467
997	293	0.658	1675	308	0.456
1102	293	0.655	1781	308	0.453
1386	293	0.638	1849	308	0.451
1509	293	0.642	1878	308	0.455
1878	293	0.629	2642	308	0.431
2642	293	0.568			
			488	318	0.420
614	298	0.585	497	318	0.378
846	298	0.595	946	318	0.400
1235	298	0.574	997	318	0.371
1253	298	0.555	1878	318	0.378
1640	298	0.545	2589	318	0.379
1665	298	0.547	2642	318	0.359
1731	298	0.553			
1871	298	0.539	497	333	0.312
1892	298	0.524	764	333	0.321
2422	298	0.510	997	333	0.310
2517	298	0.500	1287	333	0.302
2752	298	0.409	1509	333	0.324
			1878	333	0.317
625	308	0.475	2068	333	0.323
817	308	0.473	2593	333	0.317
997	308	0.466	2642	333	0.305

**Figure 3.** Diffusivity of CO₂ in water as a function of temperature.

results obtained in the present study and in Figure 4 all data are presented graphically as a function of temperature. There is a good agreement between literature results and those of the present study, thus supporting the applicability of the present experimental method. The diffusivity of N₂O in water can be calculated according to

$$D_{\text{N}_2\text{O}} = 5.07 \times 10^{-6} \exp(-2371/T) \text{ m}^2\cdot\text{s}^{-1} \quad (9)$$

3.3. Diffusivity of N₂O and CO₂ in Aqueous Alkanolamine Solutions. The diffusivity of N₂O was measured for aqueous solutions of DIPA at 293 K, DMMEA at 293 K, and MDEA at various temperatures, and these results are presented in Tables X, XI, and XII, respectively. The agreement with the data for aqueous MDEA solutions of Haimour and Sandall (6) is good

Table VII. Polynomial Coefficients for the Calculation of the Solubility of N₂O into Aqueous Alkanolamine Solutions at Various Temperatures

amine	temp, K	[amine] _{max} , mol·m ⁻³	a ₀	10 ³ a ₁ , m ³ ·mol ⁻¹	10 ⁶ a ₂ , m ⁶ ·mol ⁻²	10 ⁹ a ₃ , m ⁹ ·mol ⁻³	10 ¹² a ₄ , m ¹² ·mol ⁻⁴	10 ¹⁵ a ₅ , m ¹⁵ ·mol ⁻⁵
MEA	298	3000	0.598	0.007	-0.024	0.015	-0.003	0
DEA	298	3081	0.610	-0.026	0	0	0	0
TEA	298	2912	0.615	-0.072	-0.094	0.067	-0.013	0
DMMEA	293	2388	0.689	-0.050	0.086	-0.079	0.018	0
MDEA	293	2642	0.689	-0.005	-0.066	0.048	-0.011	0
MDEA	298	2752	0.615	-0.221	0.570	-0.606	0.266	-0.041
MDEA	308	2642	0.493	-0.022	0	0	0	0
MDEA	318	2642	0.403	-0.011	0	0	0	0
MDEA	333	2642	0.314	0	0	0	0	0
MIPA	293	3736	0.616	-0.121	0.170	-0.111	0.030	-0.003
DIPA	293	3450	0.691	-0.061	0	0	0	0
DIPA	298	4056	0.609	-0.043	-0.015	0.003	0	0
DIPA	308	2390	0.481	-0.031	0	0	0	0
DIPA	318	2390	0.397	-0.029	0	0	0	0
DIPA	333	2390	0.315	0	0	0	0	0

Table VIII. Diffusivity of CO₂ in Water at Various Temperatures

temp, K	10 ⁹ diffusivity, m ² ·s ⁻¹	ref	symbol in Figure 3
273	0.96	Tamann and Jessen (18)	□
279.5	1.15	Unver and Himmelblau (19)	○
283	1.46	Int. Crit. Tables (8)	●
288	1.60	Int. Crit. Tables (8)	●
288	1.39	Davidson and Cullen (20)	■
289	1.57	Tamann and Jessen (18)	□
291	1.71	Int. Crit. Tables (8)	●
291.5	1.65	Thomas and Adams (21)	●
292.5	1.68	Nijssing et al. (22)	⊗
293	1.64	Davidson and Cullen (20)	■
293	1.60	Taniguchi and Sakurada (23)	■
293	1.77	Int. Crit. Tables (8)	●
298	1.98	Duda and Vrentas (16)	⊙
298	1.87	Tang and Himmelblau (24)	⊕
298	1.95	Thomas and Adams (21)	●
298	2.05	Clarke (25)	■
298	1.85	Unver and Himmelblau (19)	○
298	2.00	Vivian and King (26)	×
298	1.94	Davidson and Cullen (20)	■
298	1.87	Scriven (27)	+
298	1.90	Taniguchi and Sakurada (23)	■
298	1.74	Tamann and Jessen (18)	□
303	2.29	Davidson and Cullen (20)	■
303	2.15	Taniguchi and Sakurada (23)	■
307.7	2.41	Thomas and Adams (21)	●
308	2.18	Unver and Himmelblau (19)	○
313	2.80	Duda and Vrentas (16)	⊙
318.2	3.03	Thomas and Adams (21)	●
325	3.61	Unver and Himmelblau (19)	○
327.9	3.68	Thomas and Adams (21)	●
338	4.40	Thomas and Adams (21)	●
338	4.30	Unver and Himmelblau (19)	○
348.1	5.40	Thomas and Adams (21)	●

(deviation less than 10%), which further supports the method applied here.

In order to derive a general correlation for the determination of the diffusivity of N₂O in aqueous alkanolamine solutions, the reciprocal values of the diffusivity of the data measured in the present study and those presented by Versteeg et al. (5) were multiplied by the diffusivity of N₂O in water and plotted against the ratio of the viscosity of the alkanolamine solution to water, as shown in Figure 5. (For the diffusivities, the smoothed values of the diffusivities presented in Tables X–XII and by Versteeg et al. (5) were used.) The viscosities of the various alkanolamine solutions were determined experimentally and could be approximated with relations similar to eq 6

$$\eta = a_0 + a_1[\text{amine}] + a_2[\text{amine}]^2 + \dots + a_n[\text{amine}]^n \quad (10)$$

where the polynomial coefficients are given in Table XIII.

Table IX. Diffusivity of N₂O in Water at Various Temperatures

temp, K	10 ⁹ diffusivity, m ² ·s ⁻¹	ref	symbol in Figure 4
288	1.39	Haimour and Sandall (6)	■
289.7	1.70	Davidson and Cullen (20)	○
291.1	1.47	present study	□
292	1.56	present study	□
292.9	1.48	present study	□
293	1.52	Haimour and Sandall (6)	■
293	1.92	Thomas and Adams (21)	●
293	1.74	Hufner (28)	●
293	1.45	present study	□
293	1.65	present study	□
297.9	2.09	Davidson and Cullen (20)	○
298	1.86	Haimour and Sandall (6)	■
298	1.69	Duda and Vrentas (16)	⊙
298	1.92	Joosten and Danckwerts (17)	■
298	1.78	Sada et al. (4)	■
298	1.88	present study	□
298	1.80	present study	□
302.9	2.27	present study	□
303.8	2.35	Davidson and Cullen (20)	○
308	2.03	Haimour and Sandall (6)	■
308	2.34	present study	□
312.9	2.35	present study	□
313	2.55	Duda and Vrentas (16)	⊙
313	2.58	present study	□
318	3.17	present study	□
322.7	2.85	present study	□
340	5.33	present study	□
343	5.43	present study	□
353	6.32	present study	□

Table X. Diffusivity of N₂O in Aqueous DIPA Solutions at 293 K

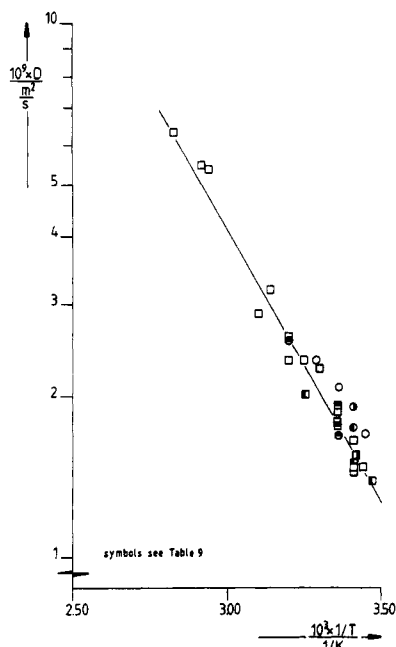
[DIPA], mol·m ⁻³	10 ⁹ D _{N₂O} , m ² ·s ⁻¹	[DIPA], mol·m ⁻³	10 ⁹ D _{N₂O} , m ² ·s ⁻¹
330	1.350	1466	0.655
505	1.450	1725	0.538
751	1.184	2222	0.331
1194	0.785		

Table XI. Diffusivity of N₂O in Aqueous DMMEA Solutions at 298 K

[DMMEA], mol·m ⁻³	10 ⁹ D _{N₂O} , m ² ·s ⁻¹	[DMMEA], mol·m ⁻³	10 ⁹ D _{N₂O} , m ² ·s ⁻¹
324	1.390	1591	0.965
611	1.235	1968	0.835
830	1.256	2049	0.714
1218	1.069	2388	0.566

From Figure 5, the diffusivity of N₂O in aqueous alkanolamine solutions at various temperatures can be calculated with the following modified Stokes–Einstein relation:

$$(D_{N_2O}\eta^{0.80})_{\text{am soln}} = \text{constant} = (D_{N_2O}\eta^{0.80})_{\text{water}} \quad (11)$$

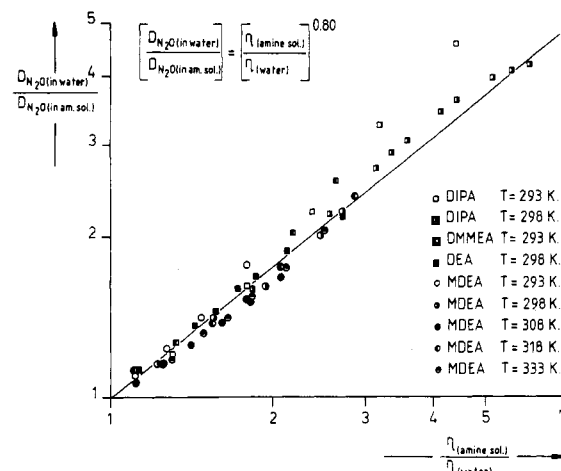
Figure 4. Diffusivity of N_2O in water as a function of temperature.Table XII. Diffusivity of N_2O in Aqueous MDEA Solutions at Various Temperatures

[MDEA], mol·m ⁻³	temp, K	$10^9 D_{N_2O}$, m ² ·s ⁻¹	[MDEA], mol·m ⁻³	temp, K	$10^9 D_{N_2O}$, m ² ·s ⁻¹
348	293	1.46	625	308	1.98
415	293	1.32	817	308	1.87
716	293	1.22	1251	308	1.64
793	293	1.16	1320	308	1.64
1102	293	1.26	1457	308	1.54
1386	293	0.81	1675	308	1.43
			1781	308	1.38
237	298	1.88	1849	308	1.31
407	298	1.32	488	318	2.46
511	298	1.44	946	318	2.18
706	298	1.36	1493	318	2.06
966	298	1.32	1985	318	1.68
1056	298	1.32	2589	318	1.47
1060	298	1.25	2865	318	1.10
1177	298	1.16			
1440	298	1.02	764	333	3.34
1591	298	1.06	1287	333	3.13
1925	298	1.64	2068	333	2.37
2056	298	0.95	2593	333	2.09
2196	298	0.77			

The deviation between eq 10 and the data of Sada et al. (4) and Haimour and Sandall (6) is always less than 20%.

Table XIII. Polynomial Coefficients for the Calculation of the Viscosity of Aqueous Alkanolamine Solutions at Various Temperatures

amine	temp, K	[amine] _{max} , mol·m ⁻³	$10^3 a_0$, m ³ ·mol ⁻¹	$10^6 a_1$, m ⁶ ·mol ⁻²	$10^9 a_2$, m ⁹ ·mol ⁻³	$10^{12} a_3$, m ¹² ·mol ⁻⁴	$10^{16} a_4$, m ¹⁶ ·mol ⁻⁵
MEA	298	3361	0.881	0.164	0.024	0	0
DEA ^a	298	5240	0.869	0.606	-0.481	0.359	-0.086
TEA	298	3500	0.898	0.200	0.449	-0.182	0.050
DMMEA	293	3690	1.001	0.262	0.175	0	0
MDEA	293	2863	1.004	0.229	0.451	-0.196	0.057
MDEA	298	3339	0.890	0.304	0.237	-0.081	0.025
MDEA	308	3339	0.719	0.198	0.210	-0.081	0.020
MDEA	318	3339	0.596	0.095	0.241	-0.101	0.020
MDEA	333	2863	0.462	0.144	0.066	-0.029	0.009
MIPA	298	3690	0.902	0.170	0.091	0	0
DIPA	293	2222	0.997	0.361	0.600	-0.249	0.102
DIPA	298	3266	0.892	0.162	0.895	-0.423	0.112
DIPA	308	3266	0.719	-0.188	1.087	-0.498	0.097
DIPA	318	3266	0.596	-0.305	1.043	-0.479	0.083
DIPA	333	3266	0.461	0.210	0.010	0.032	0

^a DEA, $a_5 = 7.8 \times 10^{-21}$ m¹⁸·mol⁻⁶.Figure 5. Stokes-Einstein plot for D_{N_2O} in aqueous alkanolamine solutions.

Therefore, the diffusivity N_2O in aqueous alkanolamine solutions can be calculated with the aid of eq 8–10 and those of CO_2 estimated with eq 7, 9, and 10.

3.4. Diffusivity of the Alkanolamine in Aqueous Alkanolamine Solutions. Hikita et al. (11, 12) presented results of the diffusivity of the alkanolamine in aqueous alkanolamine solutions at 298 K. These results were used in order to obtain a modified Stokes-Einstein relation for the diffusivity of the alkanolamine. The viscosity of the alkanolamine solution was calculated according to eq 10, the diffusivity of the alkanolamine in the solution was obtained from the smoothed results of Hikita et al. (11, 12) with the aid of an equation similar to eq 10, and the coefficients are presented in Table XIV. The diffusivity of the alkanolamine in pure water was calculated according to the methods presented by Scheibel (13), Wilke and Chang (14), and Hayduk and Laudie (15). The mean value of these three methods was taken as the diffusivity. The results of this reevaluation are presented in Figure 6 where it is concluded that the diffusivity of the alkanolamine can be estimated with the following modified Stokes-Einstein relation:

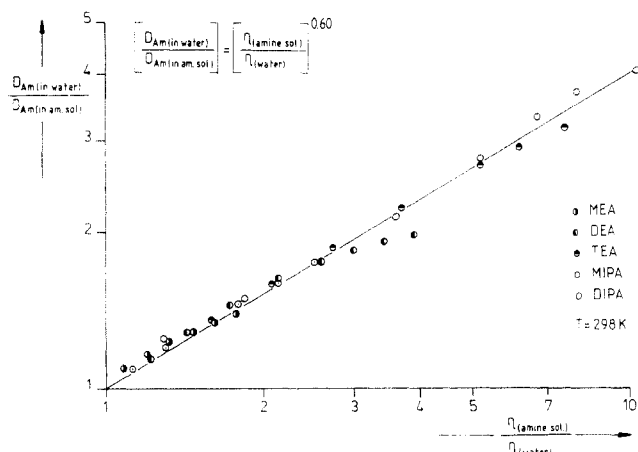
$$(D_{am}\eta^{0.60})_{am\ soln} = \text{constant} = (D_{am}\eta^{0.60})_{water} \quad (12)$$

4. Conclusions

1. With the aid of the N_2O analogy the solubility of CO_2 in aqueous alkanolamine solutions can be estimated from the ratio

Table XIV. Polynomial Coefficients for the Calculation of the Diffusivity of Alkanolamines in Aqueous Alkanolamine Solutions at 298 K

amine	[amine] _{max} , mol·m ⁻³	10 ¹⁰ a ₀ , m ² ·s ⁻¹	10 ¹³ a ₁ , m ⁵ ·mol ⁻¹ ·s ⁻¹	10 ¹⁶ a ₂ , m ⁸ ·mol ⁻² ·s ⁻¹	10 ¹⁹ a ₃ , m ¹¹ ·mol ⁻³ ·s ⁻¹	10 ²² a ₄ , m ¹⁴ ·mol ⁻⁴ ·s ⁻¹
MEA	2970	11.72	-2.426	0.784	-0.116	0
DEA	3290	8.083	-2.104	0.273	0	0
TEA	3500	7.784	-2.230	0.203	0	0
MIPA	3090	10.10	-1.866	0.145	0	0
DIPA	3370	7.358	-4.004	2.347	-0.913	0.126

**Figure 6.** Stokes-Einstein plot for D_{am} in aqueous alkanolamine solutions.

of the solubilities of CO₂ and N₂O in water in combination with the data for the solubility of N₂O in these particular solutions.

2. The diffusivity of N₂O and CO₂ in aqueous alkanolamine solutions can be calculated and estimated respectively with a modified Stokes-Einstein relation. The diffusivity of both solutes in water can be calculated with the relations presented in this study.

3. The diffusivity of the alkanolamine in aqueous alkanolamine solutions can also be calculated with a modified Stokes-Einstein relation.

Glossary

a	polynomial coefficient
C_1	constant defined by eq 1
C	concentration, mol·m ⁻³
D	diffusivity, m ² ·s ⁻¹
DEA	diethanolamine
DIPA	diisopropanolamine
DMMEA	dimethylmonoethanolamine
HE	Henry coefficient, mol·m ⁻³ ·Pa ⁻¹
m	dimensionless solubility, C_1/C_g at equilibrium, mol·mol ⁻¹
MEA	monoethanolamine
MDEA	methyldiethanolamine
MIPA	monoisopropanolamine
P	pressure, Pa
TEA	triethanolamine
η	viscosity, Pa·s

Subscripts

CO ₂	carbon dioxide
N ₂ O	nitrous oxide
am	alkanolamine
eq	equilibrium
gas	gas phase
in	initial
liq	liquid phase
water	pure water

Registry No. N₂O, 10024-97-2; CO₂, 124-38-9; DIPA, 110-97-4; MDEA, 105-59-9; DEA, 111-42-2; MIPA, 78-96-6; DMMEA, 108-01-0.

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